



# A–D–A type organic donors employing coplanar heterocyclic cores for efficient small molecule organic solar cells



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## ABSTRACT

Two linear organic A–D–A molecules (**DIPT** and **DIPTT**) comprised of electron-donating (D) coplanar heteroacenes as core end-capping with electron-accepting (A) dicyanovinylene were investigated as electron donor materials in organic photovoltaic (OPV) applications. The photophysical and electrochemical properties of these two dyes were examined. The A–D–A configuration renders these two molecules to have intense and red-shifted absorption characteristics for better light-harvesting (higher photocurrent density), while retaining relatively low HOMO energy levels for keeping sufficiently high open circuit voltage ( $V_{oc}$ ) in OPV. The optical constants and molecular orientation of thin films were acquired with variable-angle spectroscopic ellipsometry (VASE). Due to the anisotropic behavior observed in thin film, these two organic donors were firstly adopted to combine with electron acceptor  $C_{60}$  in a vacuum-processed planar heterojunction (PHJ) solar cells. The optimized **DIPT**-based PHJ device yielded a PCE of 3.01%, whereas the PHJ device based on **DIPTT**, delivered an inferior PCE of 1.70%. The exciton diffusion length extracted from spectrum-response modeling of PHJ devices is  $\sim 5$  nm and  $\sim 4$  nm for **DIPT** and **DIPTT**, respectively. Replacement of  $C_{60}$  with  $C_{70}$  for a better spectral response in 400–500 nm, planar-mixed heterojunction (PMHJ) SMOSCs without a thin donor layer in between the active layer and  $MoO_3$  was found to produce optimum device results. The optimized **DIPTT**-based device showed a PCE of 3.02%, while the shorter counterpart **DIPT** delivered a PCE up to 5.64%.

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## 1. Introduction

Organic photovoltaics (OPVs) have attracted intensive attention in recent years because of their potential advantages such as cost-effective fabrication, mechanical flexibility, color-tunable feature and low environmental impact production, which make them as promising alternatives to the conventional Si-based solar cells [1–5]. The corresponding advances in materials design [6], device architecture [7], and manufacturing process [8] have been aggressively investigated. As a result, the power conversion efficiencies (PCEs) of solution-processed bulk heterojunction (BHJ) solar cells

based on polymeric donors combined fullerene derivatives acceptors have reached remarkable PCEs over 9% [9,10]. To date, polymer-based solar cells with PCEs exceeding 10% have also been realized with tandem device structure [11–14]. Although research endeavours have been heavily invested on the polymer-based OPVs, a rapid growth in the field of small-molecule organic solar cells (SMOSCs) for the past few years has been witnessed. Small molecule-based materials offer several advantages over polymeric counterparts owing to their well-defined structure and molecular weight, easier purification, low batch-to-batch variation and better reproducibility of device performances [15,16]. Although the overall performance of SMOSCs still lags behind the polymer-based ones, some have achieved respectable PCEs beyond 8% either by vacuum- [17,18] or solution-processed [19–22] fabrication techniques. More recently, a vacuum-processed SMOSC with tandem triple-junction achieved an excellent PCE of 11% has been reported [23].

The molecular design strategy of efficient electron donors in SMOSCs generally involves the combination of electron-rich group

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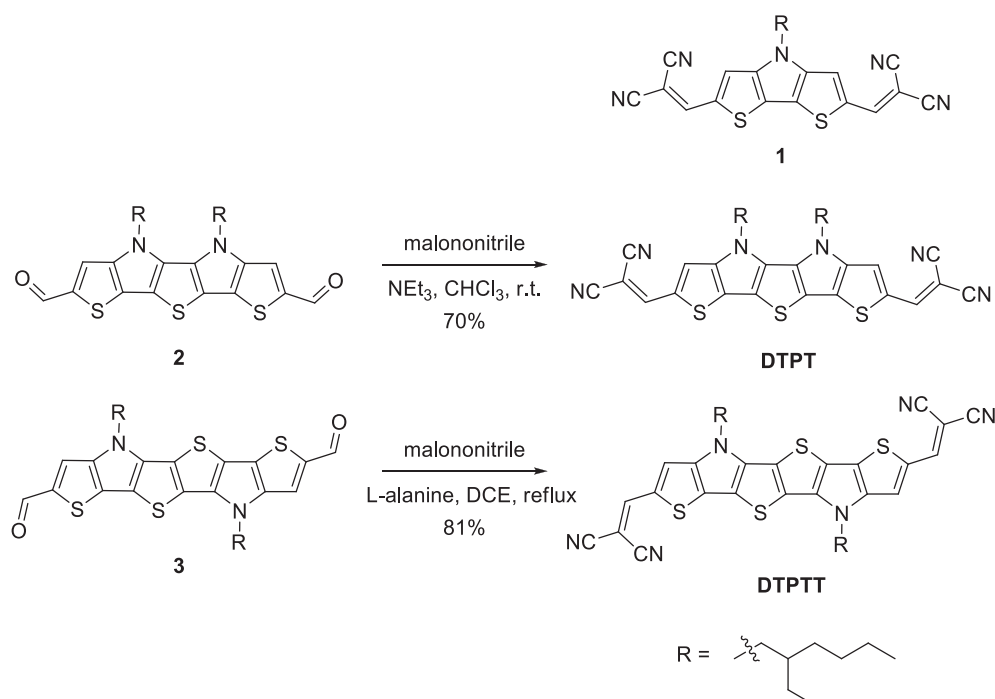
and electron-deficient group to facilitate intramolecular charge transfer (ICT). The effective ICT reduces the optical gap of molecule for extending the absorption spectrum towards longer wavelength [24–26]. Among various molecular architectures, the molecules with linear acceptor–donor–acceptor (A–D–A) configuration exhibited meritorious results in terms of photovoltaic performance [27,28]. The molecular local dipole moment within the symmetrical A–D–A scaffold can efficiently interact, leading to a diminished molecular dipolarity and less energetic disorders in bulk solid state, which is beneficial for facilitating charge carrier transport, therefore, giving better device performance [29]. Regarding to the selection of structural components for constructing an A–D–A system, dicyanovinylene (DCV) has been commonly used as strong electron-withdrawing group. Ladder-type polycyclic aromatics with fully-fused coplanar backbone are emerging as promising skeletons for making  $\pi$ -conjugated organic optoelectronic materials because of their diverse and interesting properties such as intense photoluminescence and high carrier mobility [30]. The incorporation of rigid and coplanar heteroarene into donor–acceptor system can enhance  $\pi$ -electron delocalization and elongate the effective conjugation length, resulting in a wider spectral response for giving higher photocurrent density. Moreover, it is generally believed that the stiff and coplanar molecular frameworks can suppress the conformational disorder and reduce the reorganization energy upon electron transfer, leading to enhance intrinsic charge mobility [31]. Recently, Roncali reported an A–D–A donor molecule (compound **1**, Scheme 1), in which electron-donating dithienopyrrole (DTP) was used to bridge two electron-withdrawing DCV moieties. Interestingly, molecule **1** with such short molecular length exhibits a relatively broad absorption spectrum and high molar extinction coefficient, which are useful for light harvesting. However, the photovoltaic performance (a PCE of 0.24%) obtained from a **1**-based solar cell leaves much room for improvement [32]. The common molecular design strategy for extending the spectral coverage is to increase molecular  $\pi$ -conjugation. In this regard, Bäuerle et al. reported A–D–A molecules

with  $\pi$ -extended coplanar *S,N*-heteropentacene core end-capped with electron-withdrawing groups for SMOSCs [33,34]. Stretching our previous efforts in developing dyes containing *S,N*-heterocyclic aromatic cores for dye-sensitized solar cells (DSSCs) [35], it is feasible to access analogues for probing thin film characteristics such as optical constants, molecular orientation, and exciton diffusion length. In this paper, we report two A–D–A molecules (**DTPT** and **DTPTT**), where A is DCV group and D is coplanar core *S,N*-heteropentacene and *S,N*-heterohexacene, respectively. We found that the intense and red-shifted absorption characters are responsible for better light harvesting, while the low HOMO energy levels of the donors help maximize open circuit voltage ( $V_{oc}$ ) for OPV applications. We employed the use of variable-angle spectroscopic ellipsometry (VASE) to characterize optical constants and probe molecular orientation of thin films. Both **DTPT** and **DTPTT** thin films exhibited anisotropic behavior, which is beneficial for light capture and charge transport [36]. Vacuum-processed planar heterojunction (PHJ) solar cells with **DTPT** and **DTPTT** as donor together with  $C_{60}$  as acceptor gave PCE of 3.01% and 1.70%, respectively. The exciton diffusion length extracted from the spectrum–response modeling of PHJ devices is  $\sim 5$  nm and  $\sim 4$  nm for **DTPT** and **DTPTT**, respectively. As the  $C_{60}$  acceptor was replaced with  $C_{70}$ , planar-mixed heterojunction (PMHJ) SMOSCs without a thin donor layer of **DTPTT**-based device provided a PCE of 3.02%, whereas the counterpart **DTPT** has achieved a PCE up to 5.64%.

## 2. Results and discussion

### 2.1. Synthesis of DTPT and DTPTT

Scheme 1 depicts the synthetic pathways of **DTPT** and **DTPTT**. The synthesis of the corresponding dialdehydes **2** and **3** has been reported previously [35]. Compound **2** was reacted with malononitrile to yield the target compound **DTPT** via the Knoevenagel reaction in the presence of triethylamine. The **DTPTT** with hexacyclic coplanar core was obtained in a high yield of 81% by the



**Scheme 1.** Synthetic route to **DTPT** and **DTPTT** and the structure of **1**.

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